

1-Pentanol  
71-41-0 | DTXSID6021741

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.00 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.46e-01

Confidence level: 7.81e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 2.20</div> <div>Predicted: 21.3</div>	<div>Image not found</div> <div>Methyl disulfide</div> <div>Measured: 2.45</div> <div>Predicted: 27.7</div>	<div>Image not found</div> <div>Morpholine</div> <div>Measured: 9.28e-01</div> <div>Predicted: 7.05</div>
<div>Image not found</div> <div>Barbituric acid</div> <div>Measured: 6.70</div> <div>Predicted: 4.85e-08</div>	<div>Image not found</div> <div>2,2-Dimethylbutane</div> <div>Measured: 16.0</div> <div>Predicted: 225</div>	